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Computational Studies of Novel Two-Dimensional Materials and Their Heterostructures

It has become possible in recent years to fabricate and manipulate two-dimensional nanomaterials in the laboratory that are as thin as one to few atomic layers. The reduced dimensionality gives rise to unique physical and chemical properties that differ from those of traditional bulk materials, and intriguing physical properties have been found in these few-layer systems. Computational studies have played a central role in understanding and predicting these novel properties. In this talk, I will focus on a few representative systems, including graphene systems and monolayers of transition metal dichalcogenides that exhibit properties ranging from normal semiconductors to charge density waves to superconductivity. I will report on our recent theoretical and computational studies to explore the connections among charging, lattice distortion, electronic properties, charge density waves, and superconductivity. In addition, I will discuss how the Moiré patterns in van der Waals heterostructures modify the local electronic properties and structural parameters [1,2].

References

[1] Zhang, Q. et al., Nature Communications, 7 (2016) 13843.
[2] Zhang, C. et al., Science Advances, 3 (2017) e16001459.